On-Site PFAS Detection using Spectrometry and a Machine Learning Approach

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Introduction

What are PFAS?
- Group of substances used to repel oil, grease, water, heat
- Thousands of different types of PFAS chemicals
- The most notoriously hazardous, PFOA, is studied here

Negative health effects
- Increased cholesterol
- Carcinogenic
- Fertility issues in women
- Decreased vaccine response

What are the current detection methods?
- High Resolution Mass Spectrometry (HRMS)
- Measures molecular weights
- Expensive and tedious process

Objectives

1. Design a robust portable spectrometer
2. Reliably detect PFOA
3. Train machine learning model
4. Test in the field

Novelty

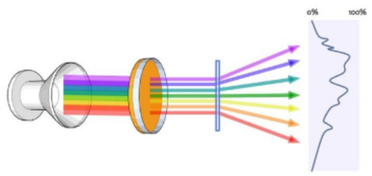
- On-site detection
- Low cost spectrometer
- The use of Hemoglobin and BSA for detection

Spectrometry

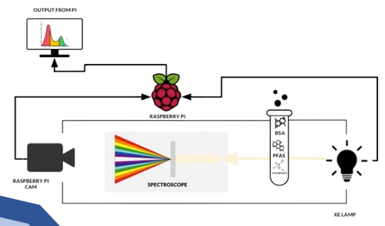
A spectrometer splits light into its individual wavelengths, and then measures the intensity of light from each wavelength.

Made of three main parts

1. Broad-Spectrum Light
2. A Diffraction Grating
3. A Camera



Design



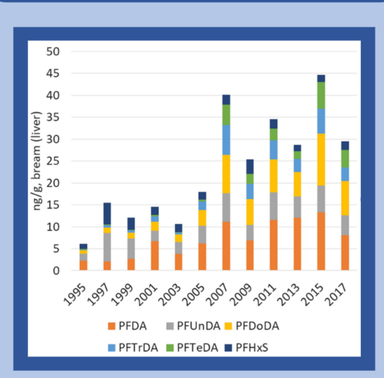
- Small 3D printed housing
- Fit with components for spectrometer
  - Raspberry Pi Zero 2 W
  - Pi Cam
  - Spectroscope
  - Broad Spectrum Light

Method

Hemoglobin & BSA
- Absorbance decreased in presence of PFOA
- Decrease in emission intensity in presence of PFOA

Both in 300 - 400nm range

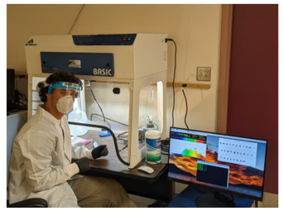
PFAS Levels Double in Freshwater Fish



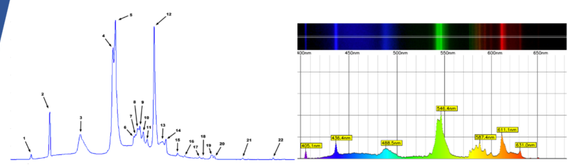
Results

- Best results were from BSA
  - Distinct change in peak wavelengths in presence of PFOA
  - New peak wavelength around 471nm
- Less significant change in hemoglobin wavelengths

Sample Type	Wavelengths						
Baseline	-	514.7nm	-	550.9nm	583.6nm	622.6nm	660nm
Hemoglobin	-	521.3nm	-	547.4nm	583.6nm	622.6nm	661.4nm
Hemoglobin 250microM PFOA	-	514.7nm	-	550.1nm	583.2nm	621.5nm	660.3nm
Hemoglobin 500microM PFOA	-	515.9nm	-	551.2nm	584nm	622.2nm	-
BSA	-	512.8nm	532.4nm	552nm	583.2nm	625.8nm	-
BSA 250microM PFOA	**471.3nm**	**508.2nm**	532nm	551.6nm	583.2nm	633.4nm	-
BSA 500microM PFOA	**471.7nm**	**510.1nm**	**541.3nm**	**562nm**	582.8nm	626.9nm	-



Calibration

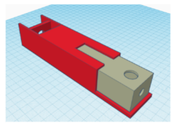


- Calibrate using fluorescent light
  - Use emission lines
- Create calibration quadratic

Build

Prototype

3D Model



Final Housing

- Adjustable to change distance of sample from camera
- Small slit to concentrate the light when it hits the cuvette
- Fit with a broad spectrum Xe bulb

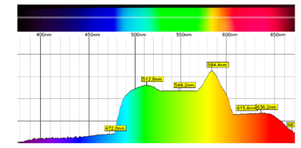
Significance

Widepread
- Found in the blood of 99% of Americans
- "Forever Chemicals"
- Found in water, soil, fish, etc

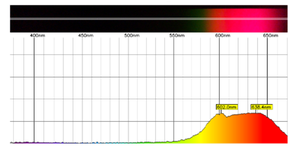
Current Pollution
- PFAS found in 21 major brands of toilet paper
- Found in 60% of 10 popular paint brands
- Used in iPhones & other cell phones until 2021
- PFAS found in every fish tested in Lake Michigan

Initial Tests

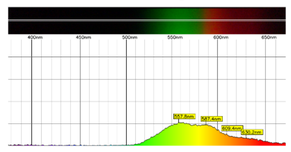
Broad Spectrum Xe Bulb



Red Dye



Green Dye



- Broad spectrum light read by spectrometer accurately
- Red dye blocks out all other light, green the same

Beer-Lambert Law

$$A = \log_{10} \frac{I_0}{I}$$

- Used to calculate the absorption of light by a solution
- A = Absorbance
- I_0 = Intensity of light transmitted through a reference sample, consisting of purely solvent
- I = Intensity of light transmitted through a sample